

Statistical Spectroscopy for Neutron-rich sd-Shell Nuclei

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ABSTRACT

Statistical spectroscopic results using the spectral distribution theory are obtained for the structure of neutron-rich light nuclei going towards the drip line and compared to experimental values available. These results will be useful for nuclear astrophysics problems where often averaged nuclear properties are adequate.

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1 Introduction

The study of neutron-rich nuclei, going right upto the drip line, with experimental results from Radioactive Ion Beam (RIB) has been immensely useful in the last couple of decades. Explaining many processes in nuclear astrophysics, like the r-process, needs the nuclear physics inputs of the neutron-rich nuclei. On the other hand the properties of the nuclei far away from stability posed a challenge to conventional models of theoretical nuclear structure and a deeper understanding of the underlying physics. However by now substantial progress has been made in building new or modifying the existing theoretical models. For the lighter nuclei shell model has been successfully used for a detailed study of the structure of the very neutron-rich nuclei [1]. It is observed that overall agreement between theoretical and experimental results are possible with adequate enlargement of the shell space and the right choice of the two body interactions and single particle wavefunctions.

Parallel to this, over the last few decades a statistical framework for nuclear spectroscopy and strength distributions of nuclear excitation and decay processes has been developed built on the original prescriptions of the use of random matrix ensembles in shell model spaces. Many reviews at different stages of its development and describing its connection to many-body quantum chaotic systems are available in literature [2] [3], [4], [5], [6], [7]. In this theory, often called the spectral distribution theory, statistically averaged forms for the nuclear level density and excitation strength distributions are obtained using arguments of random matrix ensembles and utilising the group theoretical structure of the shell model spaces, the averaged quantities are evaluated. These have the advantage of avoiding explicit diagonalisation of the Hamiltonian in many particle spaces and need to calculate traces of powers of Hamiltonian as well as their products with the excitation operators. Though these methods are suited for nuclei at excitations of a few MeV for a transition to chaos and the analytical forms obtained in the spectral distribution methods are asymptotic results, they are seen to work reasonably well even in the ground state region and for shell model spaces with not too small number of valence nucleons.

For transition strengths the detailed comparison of the spectral distribution methods with shell model has been carried out for specific *sd*-shell and *fp*-shell examples using the same two body interactions for both methods for electromagnetic and beta decay transitions [8], [9], [10], [11] and [7]. For the energy spectra one can go back to a discrete set of energy levels from the predicted averaged density of states which is continuous in energy and evaluate the binding energies of nuclei by the Ratcliff prescription [12]. A comparison with the observed binding energies for the *sd*-shell was done [13] with the Kuo interaction [14] and later [15] with the more successful Wildenthal's Universal *sd* interaction [16]. However these were carried out demonstrating the success of the spectral distributions for isotopes around the stable ones and not beyond. Similar applications for the *fp* shell nuclei were also done [17] [18] using the interaction KB3 [19] which has the monopole part properly adjusted.

These methods are expected to be useful for astrophysical applications as often the averaged strength functions and level densities are the relevant quantities there. Spectral distribution methods were earlier used for beta decay and electron capture rates during the pre-supernova evolution and subsequent gravitational collapse leading to supernova explosions [20] [21] [22].

In this letter we revisit the issue of statistical spectroscopy by spectral distribution methods in the more challenging region of very neutron-rich nuclei. We describe the calculation of the binding

energies of all neutron-rich nuclei in the sd -shell and the evaluation of occupancies and sum rule strength of a typical electromagnetic transition operator $E2$. Section 2 will discuss how well the binding energies obtained by spectral distribution methods compare with experimental values for nuclei going close to the drip line. Section 3 is involved in calculating the orbit occupancies and the isoscalar $E2$ sum rule values demonstrating how spectral distributions can describe the global features of these quantities over large excitation energies.

2 Binding Energy

It is seen that in shell model spaces with large dimensions the smoothed density of energy eigenvalues goes towards a Gaussian when the number of valence nucleons is not too small. For the non-interacting case one with a one-body Hamiltonian, one gets the result due to the operation of the Central Limit Theorem (CLT) after neglecting the Pauli blocking effect. For the interacting case i.e. with (1+2)-body Hamiltonian, the Gaussian form follows from ensemble averaging using the Embedded Gaussian Orthogonal Ensemble (EGOE) [23] [7]. With ' m ' valence particles distributed over ' N ' single particle states and with the dimension of the shell model space $d(m)$ (given by ${}^N C_m$) the normalised density of states $\rho_m(E)$ can be expressed in terms of the centroid $\epsilon(m)$ and width $\sigma(m)$. When the space is partitioned into subspaces with fixed isospin, to connect to results for real nuclei and with configuration partitioning, by distributing the ' m ' particles in ' l ' shell model orbits giving rise to the normalised configuration-isospin densities, $\rho_{\mathbf{m},T}(E)$ go to Gaussians too when each individual dimension is large enough. The intensities then just add up.

$$I_{m,T}(E) = \sum_{\mathbf{m}} I_{\mathbf{m},T}(E) = \sum_{\mathbf{m}} d(\mathbf{m}, T) \rho_{\mathbf{m},T}(E) \quad (1)$$

For almost all realistic Hamiltonians the asymptotic Gaussian results holds and the calculated higher cumulants are seen to be small.

The ground state energy E_g of a nucleus with isospin T and number of valence nucleons m is given by the Ratcliff prescription [12]

$$\sum_{\mathbf{m}} \int_{-\infty}^{\bar{E}_g} I_{\mathbf{m},T}(E) dE = d_0/2 \quad (2)$$

where d_0 is the degeneracy of the ground state. Thus the energy where the integrated area below the level density from the low energy side reaches half the degeneracy, that value is taken to be the ground state energy.

In this work we consider all nuclei with neutron number equal to or greater than the proton number, staying within the sd -shell i.e. with neutron number not exceeding 20. For locating the ground state energy more accurately we i) consider the low-lying spectrum of the nuclei and applying the Ratcliff procedure to an excited state, recover the ground state energy by subtracting the observed excitation energy from the calculated value, a procedure called 'excited state correction' here and ii) include corrections due to the small skewness and excess by incorporating the Cornish-Fisher expansion [15]. We approximate the third and fourth moments of Hamiltonian in

fixed (m, T) spaces by their scalar i.e. fixed (m) space values as presently the Spectral Distribution Method (SDM) codes calculate only the scalar 4th moments. As one goes towards neutron drip line nuclei, the experimental excitation spectra are no longer available and to compensate for this an additional isospin dependent phenomenological correction term needs to be introduced. In this letter we take that term as $0.3T^2$. In Table 1 the binding energies for the isotopes of O , F , Ne and Na calculated using SDM with Universal-sd interaction are tabulated and compared to observed values. As mentioned earlier for the success of these statistical methods the dimension of the shell model spaces should be large and that is why the nuclei having small number of valence particles or holes are not included. Table 2 gives the rest of the nuclei in the sd -shell i.e. isotopes of Mg , Al , Si , P , S , Cl and Ar , with their neutron numbers not smaller than the proton numbers. We find that overall SDM is able to reproduce the binding energies of the 70 nuclei considered reasonably well - the average deviation from the experimental values is 0.07 MeV i.e. the averaged binding energy value is slightly more than the observed one and the RMS deviation is 1.92 MeV. Figure 1 shows the calculated values compared to the observed ones for the cases of the isotopes F and Mg , two typical nuclei with odd and even proton number. One sees that for nuclei with neutron number close to or equal to 20 like ^{28}F , ^{29}Ne , ^{31}Na , ^{32}Mg and ^{33}Al the deviations of the predictions are large showing the need to enlarge the shell model space for them by including the lower fp -shell orbits like $f_{7/2}$. If one excludes these 5 nuclei the RMS deviation comes down to 1.65 MeV.

We also compare the predictions of binding energies using the A-dependent two body interaction Universal-sd with another two body interaction, Chung-Wildenthal (CW) [24]. Figure 2 gives the calculated corrected binding energies for all the neutron-rich isotopes considered for the element Ne for both interactions along with the experimental values. One sees that as one goes away from stability Universal-sd does a better job than CW, as expected.

3 Excitation Strength Sum Rule and Orbit Occupancy

Taking the density of energy eigenvalues $\rho(E)$ as the weight function one can define a unique set of orthogonal polynomials $P_\mu(E)$. If the density is Gaussian, the polynomials are Hermite. The expectation value of an operator K in the energy eigenstate $|E\rangle$ is given by

$$\langle E|K|E\rangle = \sum_{\mu} \langle KP_{\mu}(H)\rangle^m P_{\mu}(E) = \langle K\rangle^m + \zeta_{K,H}(\sigma_K)(E - \epsilon_1)/\sigma_1 + \dots \quad (3)$$

Keeping the first two terms above is called the CLT result and is seen to be true when the spectrum of the eigenvalues of H is a Gaussian and that remains so under the transformation $H \rightarrow H + \alpha K$ for small α [25]. This gives the expectation value of the operator K as a function of the energy E a geometric interpretation in terms of the correlation coefficient $\zeta_{K,H}$. if $K = O^\dagger O$ with O a one-body excitation or decay operator, then its expectation value in the state $|E\rangle$ gives the sum rule strength of excitation by the operator O . With the correlation coefficient $\zeta_{K,H}$ negative and large, the ground state region has much larger averaged strength sum than the high excitation region. On the other hand, if $\zeta_{K,H}$ has a large positive value, then the ground state region has much smaller sum rule strength than the region with high excitation energy.

Nucleus	Expt. Value (MeV)	SDM A (MeV)	SDM B (MeV)	SDM C (MeV)	SDM D (MeV)
^{21}O	-26.2	-29.3	-27.5	-27.0	-24.4
^{22}O	-32.8	-37.8	-34.7	-33.6	-30.0
^{23}O	-35.3	-39.4	-39.4	-38.0	-33.3
^{20}F	-29.9	-33.8	-31.1	-30.5	-29.9
^{21}F	-37.7	-42.2	-41.2	-39.9	-38.8
^{22}F	-42.6	-48.8	-46.1	-44.9	-43.1
^{23}F	-49.9	-55.8	-55.8	-53.5	-50.9
^{24}F	-53.5	-61.9	-59.4	-57.4	-53.8
^{25}F	-57.6	-63.2	-62.3	-60.8	-56.0
^{26}F	-58.4	-66.1	-66.1	-64.6	-58.6
^{27}F	-59.6	-65.0	-65.0	-64.5	-57.0
^{28}F	-59.2	-65.3	-65.3	-65.2	-56.2
^{20}Ne	-40.9	-40.0	-38.8	-37.4	-37.4
^{21}Ne	-47.1	-49.7	-47.5	-46.0	-45.8
^{22}Ne	-57.3	-62.9	-59.8	-57.4	-56.9
^{23}Ne	-62.1	-68.6	-66.4	-63.8	-62.7
^{24}Ne	-70.7	-80.0	-76.2	-72.6	-70.8
^{25}Ne	-74.7	-84.4	-81.1	-77.8	-75.2
^{26}Ne	-79.8	-89.8	-87.6	-84.0	-80.4
^{27}Ne	-81.0	-89.2	-89.2	-86.7	-82.0
^{28}Ne	-84.6	-92.5	-92.5	-90.5	-84.5
^{29}Ne	-85.6	-89.9	-89.9	-89.5	-82.0
^{22}Na	-58.7	-62.3	-59.1	-57.6	-57.6
^{23}Na	-70.7	-76.1	-73.3	-70.4	-70.2
^{24}Na	-77.3	-85.1	-82.8	-79.5	-78.9
^{25}Na	-86.0	-97.5	-94.1	-89.6	-88.4
^{26}Na	-91.2	-101.7	-99.0	-95.3	-93.5
^{27}Na	-97.6	-107.3	-107.3	-103.0	-100.4
^{28}Na	-100.8	-112.2	-112.2	-108.4	-104.8
^{29}Na	-110.2	-113.5	-113.5	-111.0	-106.2
^{30}Na	-107.0	-113.7	-112.1	-111.1	-105.1
^{31}Na	-110.5	-113.9	-113.9	-113.5	-106.0

Table 1: Calculated binding energies by Spectral Distribution Methods (SDM) of isotopes of O , F , Ne and Na with neutron number equal or more than the proton number, compared to experimental values. The experimental values are with respect to ^{16}O ground state and with the Coulomb part subtracted. ‘A’ refers to the Ratcliff procedure for only the ground state, ‘B’ refers to the ground state with excited state correction, ‘C’ refers to the one with excited state as well as non-zero skewness and excess and finally ‘D’ is the one which includes the isospin dependent correction to the values in column ‘C’.

Nucleus	Expt. Value (MeV)	SDM A (MeV)	SDM B (MeV)	SDM C (MeV)	SDM D (MeV)
²⁴ Mg	-87.5	-93.1	-88.9	-85.0	-85.0
²⁵ Mg	-94.4	-101.8	-98.7	-94.5	-94.3
²⁶ Mg	-105.1	-116.6	-110.7	-105.3	-104.7
²⁷ Mg	-111.2	-123.4	-119.7	-114.2	-113.1
²⁸ Mg	-119.2	-131.3	-127.1	-121.8	-120.0
²⁹ Mg	-122.6	-132.6	-131.1	-127.3	-124.7
³⁰ Mg	-128.6	-138.4	-134.8	-132.2	-128.6
³¹ Mg	-130.6	-138.5	-135.9	-134.8	-130.1
³² Mg	-136.2	-140.1	-137.6	-137.3	-131.3
²⁶ Al	-106.1	-113.7	-110.4	-106.6	-106.6
²⁷ Al	-118.7	-127.8	-124.0	-119.0	-118.8
²⁸ Al	-126.0	-137.2	-133.6	-127.9	-127.3
²⁹ Al	-135.0	-145.3	-143.1	-138.2	137.1
³⁰ Al	-140.3	-150.8	-148.1	-144.7	-142.9
³¹ Al	-147.0	-156.2	-156.2	-149.1	-146.5
³² Al	-150.9	-159.6	-155.7	-154.7	-151.1
³³ Al	-156.1	-159.5	-157.2	-156.1	-152.2
²⁸ Si	-136.0	-145.4	-141.4	-134.9	-134.9
²⁹ Si	-143.9	-155.3	-150.4	-144.8	-144.6
³⁰ Si	-154.1	-167.3	-162.8	-157.0	-156.4
³¹ Si	-160.2	-169.7	-166.7	-162.9	-161.8
³² Si	-169.0	-178.2	-175.6	-172.0	-170.2
³³ Si	-173.0	-179.0	-177.8	-176.2	-173.6
³⁴ Si	-180.2	-184.5	-183.1	-182.1	-178.6
³⁰ P	-155.5	-166.5	-161.0	-156.9	-156.9
³¹ P	-167.3	-178.5	-173.3	-169.1	-168.8
³² P	-174.7	-185.9	-181.3	-178.2	-177.6
³³ P	-184.4	-193.4	-189.5	-187.1	-186.0
³⁴ P	-190.2	-197.7	-194.9	-193.7	-191.9
³⁵ P	-198.1	-202.2	-200.6	-200.1	-197.4
³² S	-182.4	-191.6	-186.1	-182.5	-182.5
³³ S	-190.5	-198.4	-195.8	-193.2	-192.9
³⁴ S	-201.4	-209.6	-205.5	-203.3	-202.7
³⁵ S	-207.9	-213.2	-211.3	-210.3	-209.2
³⁴ Cl	-202.2	-212.4	-204.9	-203.8	-203.8
³⁵ Cl	-214.3	-219.4	-216.3	-215.4	-215.2
³⁶ Cl	-222.3	-227.2	-224.4	-224.2	-223.6
³⁶ Ar	-229.6	-232.9	-230.9	-230.1	-230.1

Table 2: Calculated binding energies by SDM of isotopes of *Mg*, *Al*, *Si*, *P*, *S*, *Cl* and *Ar* with neutron number equal to or more than the proton number, compared to experimental values. For details of the experimental values and the SDM columns ‘A’ to ‘D’ see caption of Table 1.

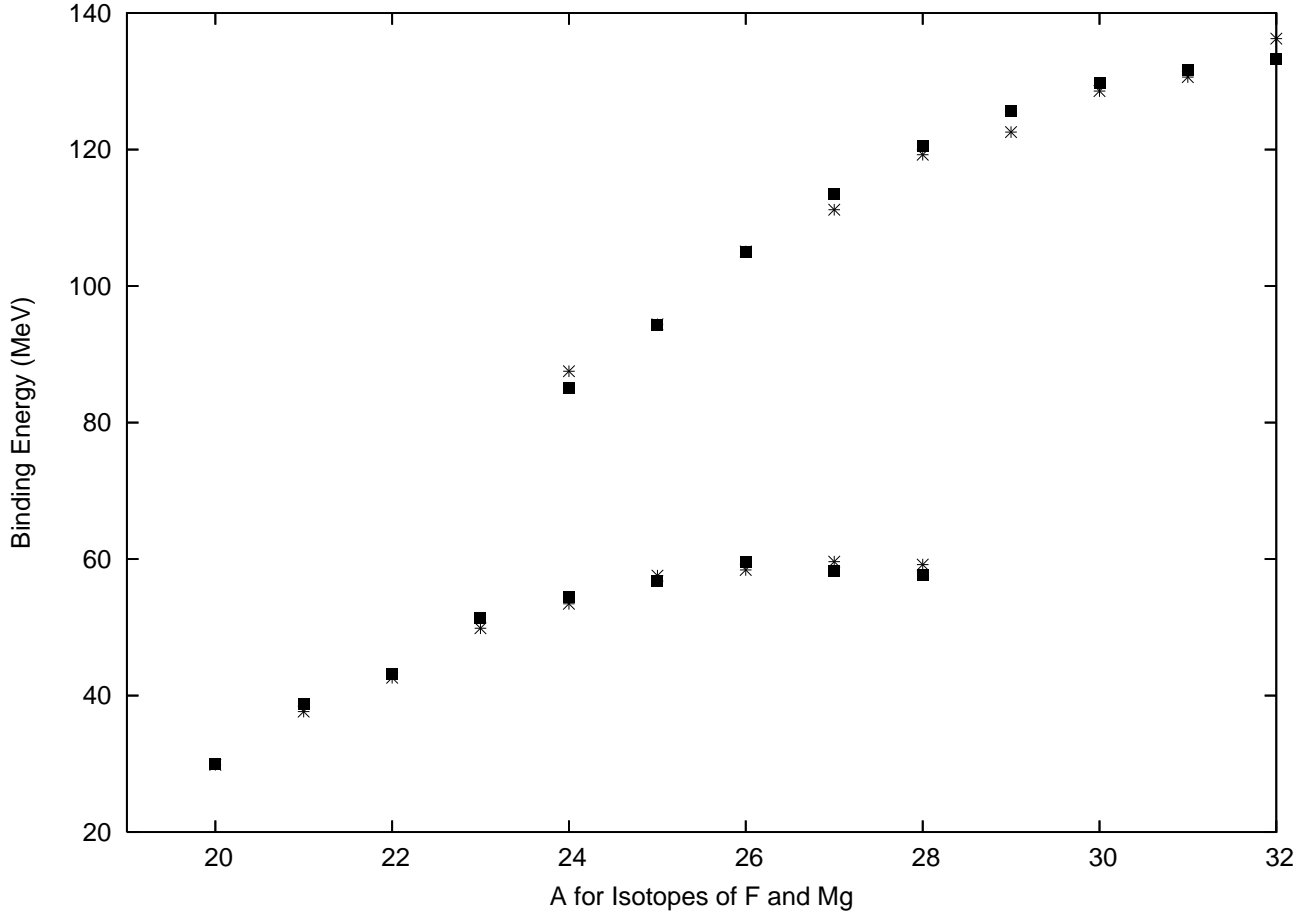


Figure 1: The absolute values of the binding energies of isotopes of F and Mg by spectral distribution methods compared to experimental values. The stars stand for the experimental values and the filled squares for the spectral distribution predictions. All the values are with respect to ^{16}O ground state energy and with the Coulomb contribution subtracted.

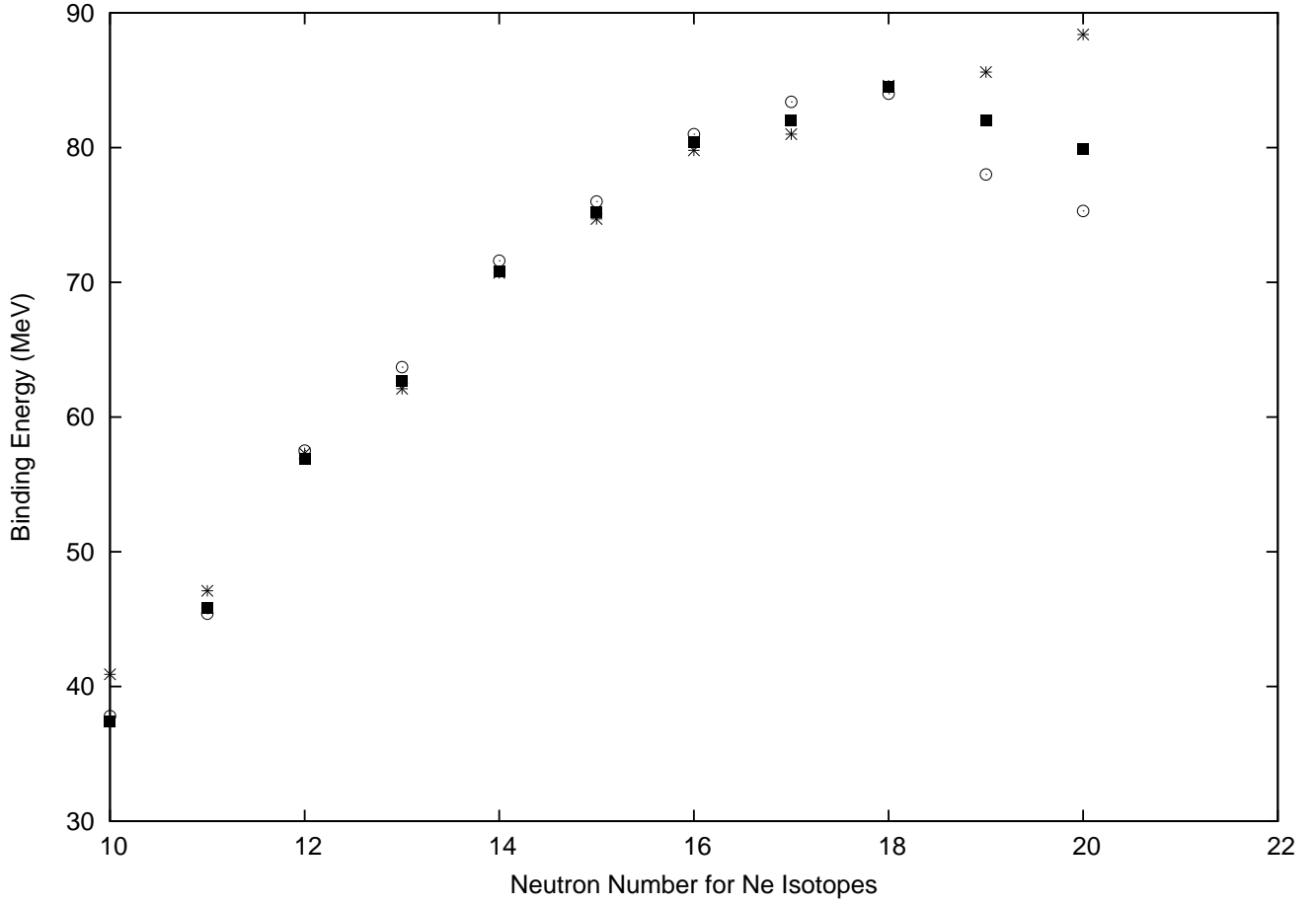


Figure 2: The absolute values of the binding energies of isotopes of Ne by the two interactions Universal-sd and CW compared to experimental values. Stars stand for the experimental numbers whereas the filled squares and the empty circles stand for the values for Universal-sd and CW interactions respectively.

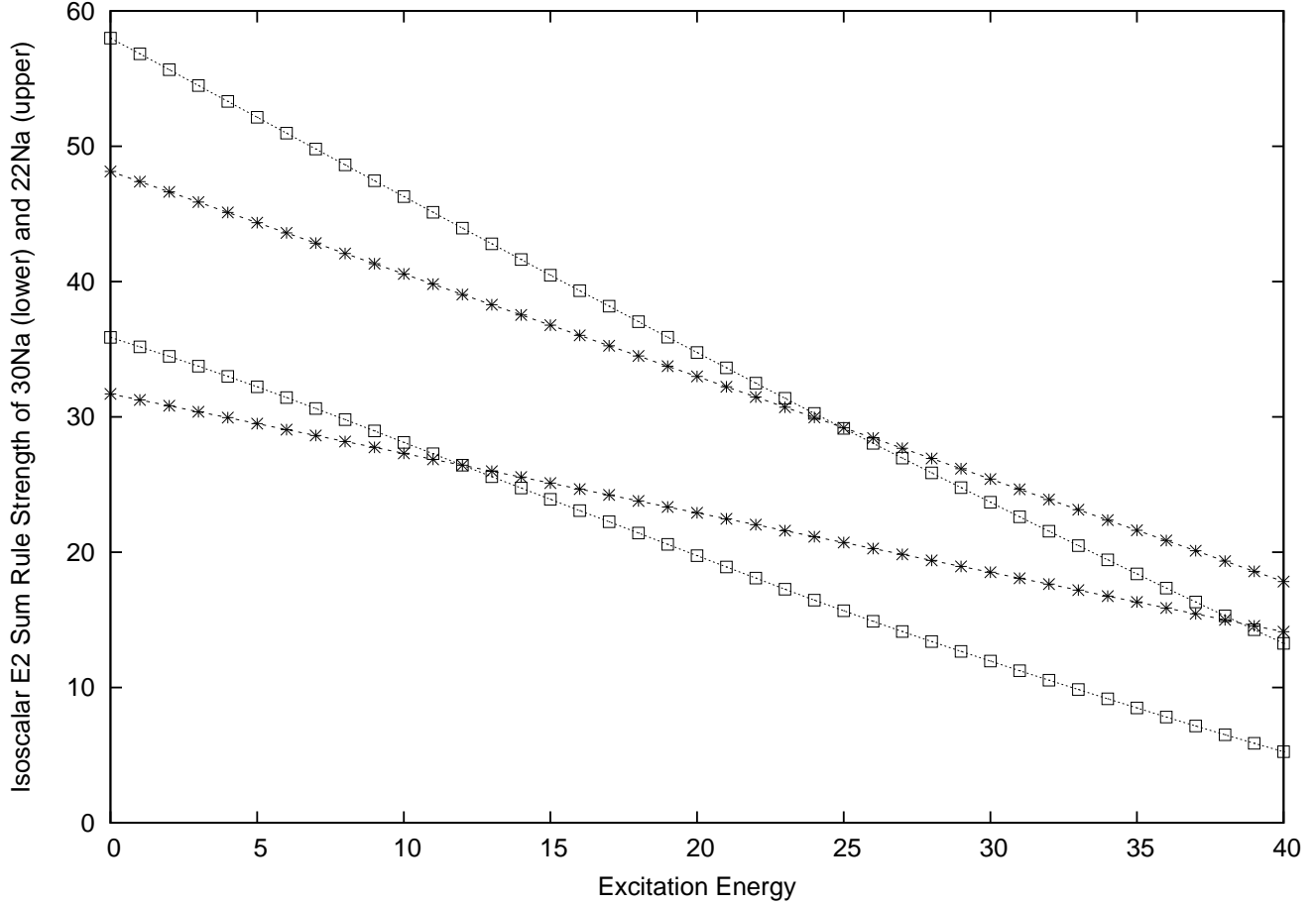


Figure 3: The sum rule strength for isoscalar E2 excitation as function of excitation energy for the nuclei ^{30}Na (the lower lines) and ^{22}Na (the upper lines) calculated by spectral distribution theory. For both nuclei the line with stars stands for the scalar result and the line with unfilled squares for the configuration result. The isoscalar E2 sum rule operator is normalized by the factor $(2.17)^2$ as done in [8].

The configuration-averaged expression for the expectation value of operator K in the energy eigenstate $|E\rangle$ for the CLT case, is

$$\tilde{K}(E)_{CLT} = \sum_{\mathbf{m}} [I_{\mathbf{m},T}(E)/I_{\mathbf{m},T}(E)] [\langle K \rangle^{\mathbf{m},T} + \tilde{\zeta}_{K,H} \tilde{\sigma}_K(E - \tilde{\epsilon}_1)/\tilde{\sigma}_1] \quad (4)$$

where $\tilde{\zeta}_{K,H}$ is the correlation coefficient between operators K and H in the configuration-isospin space (\mathbf{m}, T) along with $\tilde{\sigma}_K$, $\tilde{\epsilon}_1$ and $\tilde{\sigma}_1$ the width of K , centroid of H and width of H in the configuration-isospin space respectively.

To illustrate this we take the example of isoscalar E2 excitation for sd shell nuclei. Earlier one saw that the correlation coefficients of isoscalar E2 sum rule operator with Kuo interaction [26] with ^{17}O single particle energies [26] for a typical example of 6 particles in sd-shell are -0.52, -0.50, -0.46 and -0.36 for spaces with $T=0,1,2$ and 3 respectively [8]. We find that for the Universal-sd

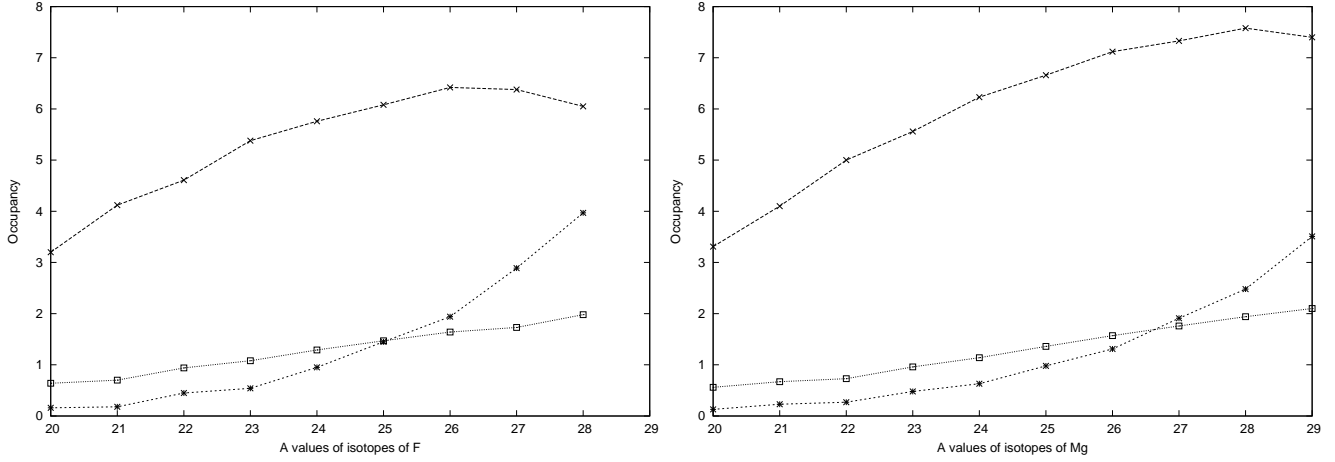


Figure 4: The predicted occupancy of isotopes of F and Mg for the three shell model orbits $d_{5/2}$, $d_{3/2}$ and $s_{1/2}$.

interaction the correlation coefficients of isoscalar E2 are -0.48 and -0.36 for the isotopes ^{22}Na (with $T=0$) and ^{30}Na (with $T=4$) respectively. Fig. 3 shows that the CLT result for the averaged isoscalar E2 sum rule strength decreases with excitation energy for the nucleus ^{22}Na with $T=0$ states as well as for the neutron-rich nucleus ^{30}Na with $T=4$ states. However the decrease is faster for ^{22}Na than for ^{30}Na . Thus this type of analysis for different excitation operators help us to understand the global features of the strength sum and strength distributions.

If one takes K as n_r , the occupancy in the shell model orbit 'r', one gets an even simpler form for the occupancy

$$n_r(E) = \sum_{\mathbf{m}} [I_{\mathbf{m},T}(E)/I_{m,T}(E)] [m_s(\mathbf{m}, T)] \quad (5)$$

where $m_r(\mathbf{m}, T)$ stands for the occupancy in the configuration-isospin space (\mathbf{m}, T) .

Thus using SDM one can easily evaluate the occupancy of all the three orbits in sd-shell for the ground state as well as the excited states. Fig. 4 gives the three ground state occupancies for the example of the isotopes of the elements F and Mg as functions of increasing mass number, A . One observes in the figure that though with the increasing value of the number of valence nucleons all three occupancies increase for both F and Mg , but the orbit $d_{5/2}$ show faster increase than the other two in the lower half of the shell. When the neutron number nears the value of 20, $d_{5/2}$ occupancy shows a decrease, stressing the need to include fp-shell orbits (at least the lowest $f_{7/2}$ orbit) in the calculation.

In conclusion, we demonstrate in this letter that the spectral distribution theory works reasonably well to reproduce global structural properties of very neutron-rich nuclei in the sd shell. This avoids the matrix diagonalisation involved in shell model and is much simpler in computation and in the interpretation of the global features than other models of nuclear structure. We plan to extend this to other excitation operators for understanding the strength distributions and sum rule strengths as well as apply this to heavier nuclei.

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